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1991 J. Phys.: Condens. Matter 3 5685

(http://iopscience.iop.org/0953-8984/3/30/002)

J. Phys.: Condens. Matter 3 (1991) 5685–5691. Printed in the UK

Local phonon properties of the Fibonacci-chain quasicrystal

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Received 4 January 1991, in final form 19 March 1991

Abstract. A new exact real-space renormalization group approach is presented for the local phonon properties of any given site in an infinite Fibonacci chain. It is found that the local phonon densities of states for different sites are different from each other, although they have the same structure. Results also suggest that the local phonon spectrum is a Cantor set.

1. Introduction

As a one-dimensional (1D) analogue of the Penrose tiling, the Fibonacci chain has been studied in great detail in recent years. For the electronic and phonon properties of this quasiperiodic system, it is well known that [1–8] the global spectrum for each case is a Cantor set, i.e. the spectrum has self-similarity and the gaps in the spectrum are distributed densely. On the other hand, to our knowledge, most work on the spectrum of the Fibonacci chain is mainly devoted to the analysis of the global structure of the spectrum and not much attention has been paid to study of the local properties. Naturally, because there is no translational symmetry in the Fibonacci chain, each site has a different environment, but the case is not the same as that of the random system because of the existence of the long-range order of the Fibonacci chain. So it is essential to develop a method to investigate the local properties of this quasiperiodic system. Recently, the computation of the local density of states (LDOS) at a particular site of the Fibonacci chain was first performed by Ashraff and Stinchcombe [9] and later by Chakrabarti *et al* [10] based on the decimation scheme first used by Southern *et al* [11] and Goncalves da Silva and Koiller [12]. However, in our judgment, so far no powerful method has been found to obtain the LDOS at any site. For this reason, we develop a new real-space renormalization group (RSRG) scheme here to study the local electronic and phonon properties of an infinite Fibonacci chain. It will be seen that our scheme is convenient and powerful in studying the local Green function (LGF) and the LDOS at any given site. In this paper, we mainly study the phonon problem. We shall discuss the electronic case elsewhere [13].

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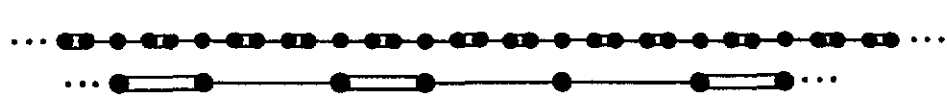

Figure 1. A schematic representation for the basic transformation T_α on a Fibonacci chain.

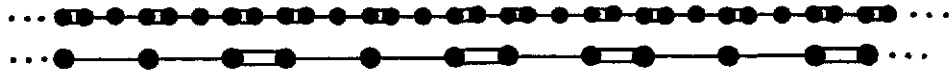

Figure 2. A schematic representation for the basic transformation T_β on a Fibonacci chain.

2. A renormalization group scheme for the local Green functions

Study of the excitation spectrum of electrons and phonons in the Fibonacci chain often starts from a 1D tight-binding Hamiltonian as follows:

$$H = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{ij} |i\rangle V_{ij} \langle j| \tag{1}$$

where each state $|i\rangle$ is an atomic-like orbital centred at site i, and ε_i and V_{ij} denote the diagonal and off-diagonal matrix elements of the Hamiltonian in this basis, in which V_{ij} takes two values V_A and V_B arranged in a Fibonacci sequence which is constructed by the inflation rule $(A, B) \rightarrow (AB, A)$ and ε_i takes one of the following three values according to the local environment of site i:

$$\varepsilon_i = \begin{cases} \varepsilon_\alpha \\ \varepsilon_\beta \\ \varepsilon_\gamma \end{cases} \quad \text{if} \begin{cases} V_{i-1,i} = V_{i,i+1} = V_A \\ V_{i-1,i} = V_A \text{ and } V_{i,i+1} = V_B \\ V_{i-1,i} = V_B \text{ and } V_{i,i+1} = V_A. \end{cases}$$

From equation (1) it follows that the matrix elements of the Green function $G_{ij} = \langle i|G|j\rangle$ satisfy the following set of equations:

$$(Z - \varepsilon_i)G_{ij} = \delta_{ij} + \sum_k V_{ik} G_{kj} \qquad i, j = 0, \pm 1, \pm 2, \ldots \tag{2}$$

where $Z = E + i0^+$ and δ_{ij} is the Kronecker delta. The LDOS at site i is then given by the diagonal element of the Green function

$$\rho_i(E) = -(1/\pi)\,[\mathrm{Im}\, G_{ii}(E + i0^+)] \tag{3}$$

where Im denotes the imaginary part of a complex.

2.1. Three basic renormalization transformations

In order to obtain the LGF at any given site, we introduce three basic renormalization transformations T_α, T_β and T_γ according to the self-similar structure of the Fibonacci chain. If the nearest-neighbour interactions are considered, all the sites in the Fibonacci chain can be divided into three types denoted by type α, type β and type γ with site

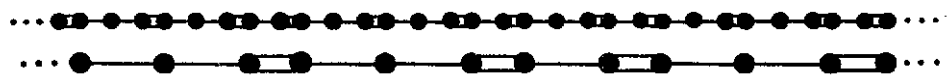

Figure 3. A schematic representation for the basic transformation T_γ on a Fibonacci chain.

energies ε_α, ε_β and ε_γ, respectively. Transformations T_α, T_β and T_γ illustrated in figures 1–3 are the decimations for sites of different types.

2.1.1. Transformation T_α. All sites belonging to type β and type γ are decimated, while sites of type α with renormalized parameters form a new Fibonacci chain (figure 1). This procedure can be represented by $(ABABA, ABA) \rightarrow (A', B')$ and the corresponding RG equations are

$$\begin{aligned}
\varepsilon'_\alpha &= \varepsilon_\alpha + W + V_A^2/(E-X) + [V_B^2 W/Y(E-\varepsilon_\beta)][1 + V_A^2/(E-X)^2] \\
\varepsilon'_\beta &= \varepsilon_\alpha + W + [1/(E-X)][V_A^2 + V_B^2 W/(E-\varepsilon_\beta)] + V_A^2 V_B^2 W/Y(E-X)^2(E-\varepsilon_\beta) \\
\varepsilon'_\gamma &= \varepsilon_\alpha + W + V_A^2/(E-X) + V_B^2 W/Y(E-\varepsilon_\beta) \\
V'_A &= V_A V_B^2 W/Y(E-X)(E-\varepsilon_\beta) \\
V'_B &= V_B W/(E-X)
\end{aligned} \tag{4}$$

where

$$\begin{aligned}
W &= V_A^2/(E-\varepsilon_\beta) \\
X &= \varepsilon_\gamma + V_B^2/(E-\varepsilon_\beta) \\
Y &= E - \varepsilon_\gamma - (V_A^2 + V_B^2)/(E-\varepsilon_\beta) - V_A^2 V_B^2/(E-X)(E-\varepsilon_\beta)^2.
\end{aligned} \tag{5}$$

2.1.2. Transformation T_β. The decimated sites are sites of type α and type γ, and the new Fibonacci chain is composed of sites of type β in the original chain (figure 2). T_β can be represented by $(BAA, BA) \rightarrow (A', B')$ and its RG equations are

$$\begin{aligned}
\varepsilon'_\alpha &= \varepsilon_\beta + P + [V_A^2/(E-Q)][1 + P/(E-\varepsilon_\gamma)] \\
\varepsilon'_\beta &= \varepsilon_\beta + P + V_A^2/(E-Q) \\
\varepsilon'_\gamma &= \varepsilon_\beta + P + [V_A^2/(E-\varepsilon_\gamma)][1 + P/(E-Q)] \\
V'_A &= V_A^2 V_B/(E-Q)(E-\varepsilon_\gamma) \\
V'_B &= V_A V_B/(E-\varepsilon_\gamma)
\end{aligned} \tag{6}$$

where

$$\begin{aligned}
P &= V_B^2/(E-\varepsilon_\gamma) \\
Q &= \varepsilon_\alpha + V_A^2/(E-\varepsilon_\gamma).
\end{aligned} \tag{7}$$

2.1.3. Transformation T_γ. For this transformation represented by $(AAB, AB) \rightarrow (A', B')$, the new Fibonacci chain comes from the sites of type γ of the original chain, while the corresponding RG equations can be obtained immediately by interchanging the subscripts β and γ in equations (6) and (7).

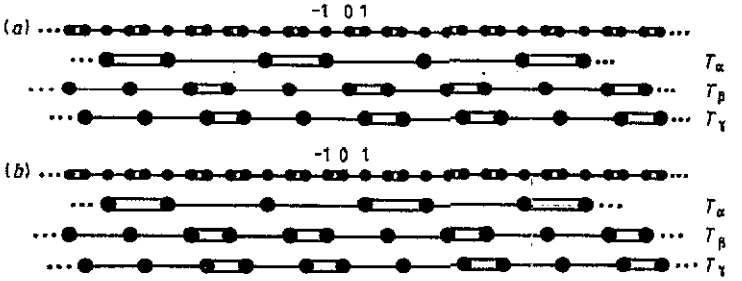

Figure 4. Transformations T_β and T_γ classify the Fibonacci chains of different generations into two classes with key sites of different types, while the nearest-neighbour sites of the key site can be transferred to the key sites by suitable combinations of T_α, T_β and T_γ: (*a*) a Fibonacci chain with key site (site 0) of type S_β; (*b*) a Fibonacci chain with key site (site 0) of type S_γ.

From the above statements for the transformations T_α, T_β and T_γ, we have the following conclusions. If we apply T_α, T_β and T_γ to a Fibonacci chain individually, three renormalized Fibonacci chains are obtained. The sites of the original chain are all converted to these new chains. In the asymptotic limit, the length scale factors of the transformations T_β and T_γ are τ^2, while the length scale factor for the transformation T_α is τ^3, where τ is the golden mean.

2.2. Local Green function at any site

We consider Fibonacci chains of different generations. A careful examination of the transformations T_β and T_γ shows that every Fibonacci chain has a special site which we call the key site. The key site has the properties that, through the transformation T_β or T_γ, it remains undecimated while the local environment of this site in the new Fibonacci chain is the same as that in the original one. We illustrate this property in figure 4. There is only one key site for a Fibonacci chain. These key sites are divided into two types denoted by type S_β and S_γ according to the corresponding transformations T_β and T_γ, respectively. Therefore Fibonacci chains of different generations can be classified into two distinct classes by the different types of key site. No successive generations belong to the same class. The LGF at the key site of type S_β or S_γ in an infinite Fibonacci chain can be obtained by successive iterations of the transformation T_β or T_γ. Since V_A and V_B approach zero by successively iterating T_β or T_γ, there is only a 'pseudoatom' with energy ε_β^* or ε_γ^* after infinite iterations, and the LGF at the key site of type S_β or S_γ is then given by

$$G_{00} = 1/(E - \varepsilon_\beta^*) \tag{8}$$

or

$$G_{00} = 1/(E - \varepsilon_\gamma^*) \tag{9}$$

where we assume that the origin of the chain is the position of the key site.

Now we focus our attention to the calculations of the LGF at other sites. We first assume that the key site is type S_β and denote it as site 0. It is found that T_γ makes site 1 become the key site of type S_β in the new Fibonacci chain, while T_α makes site -1 become the key site of type S_γ (figure 4(*a*)). If site 0 is the key site of type S_γ, we find

that site -1 is transferred to the key site of type S_γ by T_β, while site 1 is transferred to the key site of type S_β by T_α (figure 4(*b*)). So the problem of the calculation of the LGF at a site which is the nearest-neighbour site of the key site becomes the problem of the key site. We repeat the same procedure for each new chain obtained by performing T_α, T_β and T_γ and in this way we can convert any other given site to a key site in a renormalized Fibonacci chain and obtain the corresponding LGF. For example, the LDOSS at site 2(-2), 3(-3), 4(-4) . . . are given by the transformations $T_\beta T_\gamma T_\beta T_\beta T_\beta \ldots (T_\gamma T_\alpha T_\gamma T_\gamma T_\gamma \ldots)$, $T_\gamma T_\gamma T_\beta T_\beta T_\beta \ldots (T_\beta T_\alpha T_\gamma T_\gamma T_\gamma \ldots)$, $T_\alpha T_\alpha T_\beta T_\beta T_\beta \ldots (T_\alpha T_\beta T_\gamma T_\gamma T_\gamma \ldots)$, . . . , respectively, for the original chain with key site of type S_β, while the LDOSS at these sites in the original chain with key site of type S_γ are given by the transformations $T_\beta T_\alpha T_\beta T_\beta T_\beta \ldots (T_\gamma T_\beta T_\gamma T_\gamma T_\gamma \ldots)$, $T_\gamma T_\alpha T_\beta T_\beta T_\beta \ldots (T_\beta T_\beta T_\gamma T_\gamma T_\gamma \ldots)$, $T_\alpha T_\gamma T_\beta T_\beta T_\beta \ldots (T_\alpha T_\alpha T_\gamma T_\gamma T_\gamma \ldots)$, . . . , respectively.

3. Local phonon density of states

The phonon problem of the 1D quasiperiodic system is usually described by the following equation of motion:

$$-\omega^2 \psi_i = K_{i+1}\psi_{i+1} + K_i \psi_{i-1} - (K_{i+1} + K_i)\psi_i \tag{10}$$

where ψ_i denotes the displacement of the ith atom from its equilibrium position and K_i takes two values K_A and K_B which are arranged in the Fibonacci sequence. Equation (10) can be rewritten as

$$[\omega^2 - (K_{i+1} + K_i)]\psi_i = -K_{i+1}\psi_{i+1} - K_i \psi_{i-1}. \tag{11}$$

Comparing (11) with the tight-binding model for the electronic problem

$$(E - \varepsilon_i)\psi_i = V_{i+1}\psi_{i+1} + V_i \psi_{i-1} \tag{12}$$

we obtain a Hamiltonian with the same form as equation (1). The parameters are

$$\varepsilon_i = \begin{cases} 2K_A \\ K_A + K_B \\ K_B + K_A \end{cases} \qquad \text{if} \begin{cases} K_{i-1,i} = K_{i,i+1} = K_A \\ K_{i-1,i} = K_A \text{ and } K_{i,i+1} = K_B \\ K_{i-1,i} = K_B \text{ and } K_{i,i+1} = K_A \end{cases}$$

$V_A = -K_A$ and $V_B = -K_B$, while E is replaced by ω^2.

Now we can study the local phonon properties using the RSRG scheme described in section 2. The LDOSS at several sites are given in figures 5–7, where site 0 is the key site of type S_β. In figures 5(*a*) and 5(*b*) we present the results for site 0 and site 2, respectively. Figures 6(*a*) and 6(*b*) are devoted to site 1 and site 3, while figures 7(*a*) and 7(*b*) correspond to site -1 and site 4. When nearest-neighbour interactions are considered, site 0 and site 2 are sites of type β, site 1 and site 3 belong to type γ, and site -1 and site 4 are sites of type α. One can see from figures 5–7 that the spectrum for every site is composed of three main clusters, and each of these consists of three subclusters. Such a trifurcating structure which is more explicit in the high-frequency region indicates that the spectrum is self-similar. In addition, the behaviours of K_A and K_B show that the eigenfrequencies are discrete because K_A and K_B approach zero under the transformations for all real or complex E. All this suggests that the local phonon spectrum is a Cantor set. Sire and Mosseri [14] have studied the behaviour of the gap widths of a

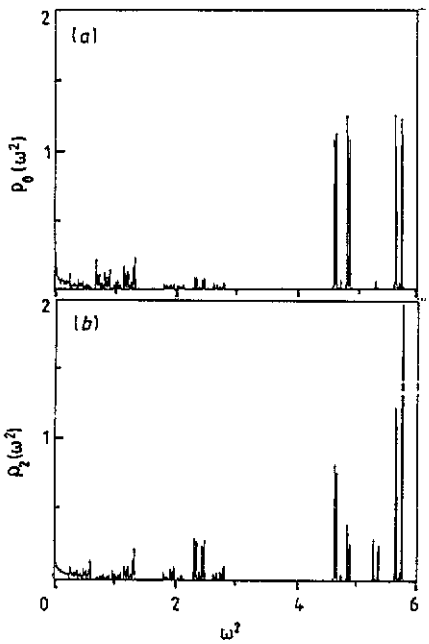

Figure 5. The LDOSS (arbitrary units) at two sites of type β, in which $K_A = 1$ and $K_B = 2$: (*a*) site 0 (key site of type S_β); (*b*) site 2.

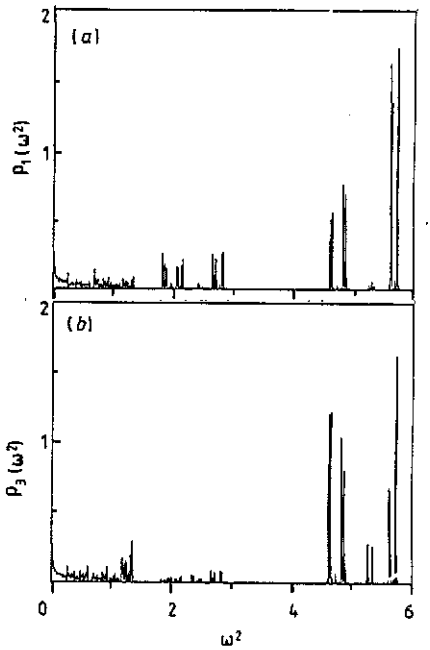

Figure 6. The LDOSS (arbitrary units) at two sites of type γ, in which $K_A = 1$ and $K_B = 2$: (*a*) site 1; (*b*) site 3.

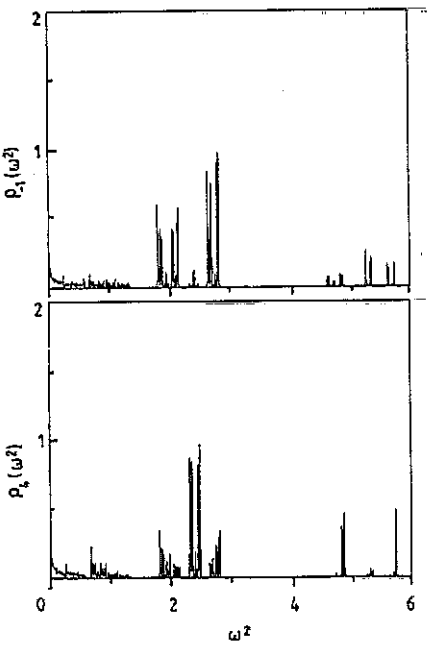

Figure 7. The LDOSS (arbitrary units) at two sites of type α, in which $K_A = 1$ and $K_B = 2$: (*a*) site -1; (*b*) site 4.

quasiperiodic Hamiltonian. Their results showed that, at weak frequencies, the local integrated density of states (LIDOS) at a sufficiently weak potential is equivalent to the IDOS of the periodic strain chain and the LIDOSs at different sites are equal in the limit $\omega \to 0$ for the general case. Careful examination of figures 5–7 shows that our results are not in conflict with the above conclusions. Another feature concerning the local phonon properties is that, on the one hand, the LDOSs for different sites are different from each other even though there may be the same nearest-neighbour interactions but, on the other hand, the LDOSs have the same structure.

4. Summary

We have given a new RSRG scheme to study the local phonon properties of an infinite Fibonacci chain. In our RSRG scheme, three basic renormalization transformations T_α, T_β and T_γ are introduced. Transformations T_β and T_γ classify the Fibonacci chains of different generations into two classes with key sites of type S_β and type S_γ, respectively. No successive generations belong to the same class. Any other site can be transferred to the key site of a renormalized Fibonacci chain by suitable combinations of T_α, T_β and T_γ. The LDOS at the key site of type S_β or S_γ is obtained by successive iterations of the transformation T_β or T_γ. Numerical results show that the LDOSs for different sites are different from each other, although they have the same structure. In addition, we find that the local phonon spectrum is a Cantor set. All these observations indicate that the local phonon properties of the Fibonacci chain are between the periodic system and the random system, just as the characteristic of the structure of the Fibonacci chain is.

Acknowledgments

We would like to thank one of the referees for helpful suggestions. This work has been supported by the National Natural Science Foundation of China and in part by CCAST (World Laboratory).

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